

Finite-temperature phase transition in a homogeneous one-dimensional gas of attractive bosons

Christoph Weiss*

Joint Quantum Centre (JQC) Durham–Newcastle, Department of Physics,
Durham University, Durham DH1 3LE, United Kingdom

(Dated: Submitted: August 16, 2013; current version October 29, 2016)

In typical one-dimensional models the Mermin-Wagner theorem forbids long range order, thus preventing finite-temperature phase transitions. We find a finite-temperature phase transition for a homogeneous system of attractive bosons in one dimension. The low-temperature phase is characterized by a quantum bright soliton without long range order; the high-temperature phase is a free gas. Numerical calculations for finite particle numbers show a specific heat scaling as N^2 , consistent with a vanishing transition region in the thermodynamic limit.

PACS numbers: 05.70.Fh, 03.75.Lm, 05.30.Jp, 03.75.Hh

Keywords: phase transition, one dimension, finite temperatures, bright solitons, Bethe ansatz, Lieb-Liniger model, attractive interactions, Mermin-Wagner theorem, Bose-Einstein condensation

Bright solitons generated from attractively interacting Bose-Einstein condensates in quasi-one-dimensional wave guides are investigated experimentally in an increasing number of experiments[1–10]. As experiments do not truly take place in one dimension but rather in *quasi*-one-dimensional wave guides, providing a thermalization mechanism [11, 12], this leads to the question whether or not these bright solitons can be stable in the presence of thermal fluctuations.

The Mermin-Wagner theorem [13] proves that in many models long-range order in one or two dimensions cannot exist at finite temperatures [13, 14]; this excludes the existence of many phase transitions. Finite-temperature transitions are fundamentally different from quantum phase transitions (cf. [15, 16]); one-dimensional quantum phase transitions can be found, e.g., in Refs. [17–19]). While there are some finite temperature phase transitions in low-dimensional systems like the Berezinsky-Kosterlitz-Thouless transition in two dimensions [20] or the phase transition in the two-dimensional Ising model [21], the generic case is that low-dimensional models do not undergo finite-temperature phase transitions [22]. Indeed, a book on “thermodynamics of one-dimensional *solvable* models” does not include the word “phase transition” in its index [23]. For a *disordered* system displaying Anderson-localization [24], a finite-temperature phase transition for weakly interacting bosons in one dimension has been found in Ref. [25].

A quasi one-dimensional system of attractively interacting bosons can be modeled [26–29] by the *solvable* Lieb-Liniger model [30–32]. One of the challenges for bright-soliton experiments [1–7, 33] is to realize true quantum behavior predicted, so far, with zero-temperature calculations [34–40]. For the Lieb-Liniger model, investigations of thermal effects on the many-body level for bosons in one dimension have so far focused on the more extensively studied case of repulsive interactions (Ref. [23] and references therein); for finite systems classical field methods have been applied [41]. In other soliton models, thermodynamics with interacting solitons has been investigated [42, 43].

In this Letter we show that attractive bosons in the Lieb-Liniger model undergo a finite-temperature phase transition;

a bright soliton – no-soliton transition. As bright solitons do not display long-range order, this does not violate the Mermin-Wagner theorem. Although bright solitons do not display long-range order, quantum bright solitons are fundamentally different from localized states cf. [25]: For the Lieb-Liniger model, the energy eigenfunction describing a soliton of N -particles has to obey the symmetry of the Hamiltonian and is thus translationally invariant.

For N identical bosons on a one-dimensional line of length L , corresponding to the experimentally realizable [44] box potential, the Lieb-Liniger Hamiltonian reads [30–32]

$$\hat{H} = - \sum_{j=1}^N \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_j^2} + \sum_{j=1}^{N-1} \sum_{n=j+1}^N g_{1D} \delta(x_j - x_n),$$

where $g_{1D} < 0$ quantifies the contact interactions between two particles, m is the mass, and x_j the position of the j th particle. Contrary to the phenomenological model used in [45] for a harmonically trapped one-dimensional gas of attractive bosons, we use the complete set of energy-eigenvalues which are known analytically for large L ¹ [27, 46],

$$E_{LL}(\{n_r, k_r\}_{r=1\dots R}) = \sum_{r=1}^R \left(E_0(n_r) + \frac{\hbar^2 K_r^2}{2n_r m} \right), \quad \sum_{r=1}^R n_r = N, \quad (1)$$

where the R natural numbers n_r correspond to either free particles, if $n_r = 1$, or matter-wave bright solitons, if $n_r > 1$ (cf. the energy-eigenfunctions discussed in Ref. [27]; for experiments with more than two solitons see Refs. [2, 3], cf. [34, 38]). Each soliton has kinetic energy (proportional to the square of the single-particle momentum $\hbar k_r$, shared by all particles belonging to this soliton) and ground-state energy [27, 31]

$$E_0(n_r) = -\frac{1}{24} \frac{mg_{1D}^2}{\hbar^2} n_r (n_r^2 - 1). \quad (2)$$

¹ The precise limit, which was not discussed in Refs. [30, 31], will be defined in Eq. (4) after the necessary physical requirements on this limit are stated.

We choose periodic boundary conditions (cf. [46]) which lead to KL having to be an integer multiple of 2π , thus

$$K_r = \frac{2\pi}{L} \nu_r, \quad \nu_r = \dots, -2, -1, 0, 1, 2, \dots$$

As we are dealing with indistinguishable particles, many-particle wave functions [27] are unambiguously defined by only considering configurations with

$$n_1 \geq n_2 \geq n_3 \geq \dots \geq n_R.$$

Because of Eq. (1), the total number of possibilities to distribute N particles among up to N parts is thus given by the number partitioning problem [47]

$$p(N) \sim \frac{1}{4N\sqrt{3}} \exp\left(\frac{\pi\sqrt{2}}{\sqrt{3}} \sqrt{N}\right), \quad N \gg 1. \quad (3)$$

The $\propto N^3$ -dependence of the ground-state energy (2) is a problem for the treatment of the thermodynamic limit ($N \rightarrow \infty$, $L \rightarrow \infty$ such that $N/L = \text{const.}$) [23]; the Lieb-Liniger model with repulsive interaction is thus normally used to do thermodynamics [23]. However, for attractive interactions treating the limit $N \rightarrow \infty$ at fixed interaction would lead to infinite densities, cf. [27]. We thus combine the thermodynamic limit with vanishing interaction – as used in the mean-field (Gross-Pitaevskii) theory of bright solitons [48].

$$N \rightarrow \infty, \quad L \rightarrow \infty, \quad g_{1D} \rightarrow 0, \quad \varrho = \text{const.}, \quad \tilde{g} = \text{const.}, \quad (4)$$

where $\varrho \equiv N/L$ and $\tilde{g} \equiv Ng_{1D}$. When approaching the limit (4), the energy-gap $E_{\text{gap}} \equiv E_0(N-1) - E_0(N)$ is an N -independent energy scale which will turn out to be the relevant energy scale for thermodynamics; we can express characteristic temperatures as

$$k_B T_0 = A E_{\text{gap}}; \quad (5)$$

and subsequently investigate if the prefactor A remains non-zero in the limit (4). The ground state energy (2) now reads

$$E_0(n_r) = -\frac{E_{\text{gap}}}{3N(N-1)} n_r(n_r^2 - 1);$$

in the limit (4) the energy gap is given by

$$E_{\text{gap}} = \frac{1}{8} \frac{m\tilde{g}^2}{\hbar^2} = \text{const.} > 0.$$

Before we choose the *canonical ensemble* (characterized by temperature T and particle number N [49]) to do thermodynamics, we should quantify the requirement that L has to be large in order for the energy-eigenvalues (1) to be correct within the limit (4). The ground-state wave function for N bosons is given by $\psi_0 \propto \exp[-m|g_{1D}|/(2\hbar^2) \sum_{1 \leq j < n \leq N} |x_j - x_n|]$; the size of an N -particle soliton $\sigma \propto 1/(|g_{1D}|N)$ [27] and thus remains a non-zero constant in the limit (4), leading to a single particle density $\propto \cosh(x/\sigma)^{-2}$ and thus also to a vanishing

off-diagonal long-range order.² In order for the energy eigenvalues given by Eq. (1) to be valid, the system has to be larger than the size of a $N = 2$ soliton (the more particles are in a soliton, the smaller it gets [27]). To be on the safe side we ask the wave function to be below e^{-100} for particle separation greater than L , that is

$$\frac{m|g_{1D}|}{2\hbar^2} L \gtrsim 100.$$

For the two relevant energy scales of Eq. (1) this gives an energy ratio

$$\begin{aligned} \mathcal{E}(N) &\equiv \frac{E_{\text{gap}}}{E_{n_r=1, \text{kin}}(\nu_r=1)} = BN^2, \\ B &\equiv \left(\frac{mg_{1D}}{2\hbar^2} L\right)^2 \frac{1}{(2\pi)^2}; \end{aligned} \quad (6)$$

the eigenvalues (1) are therefore a very good approximation to the true eigenvalues of the Lieb-Liniger model (for all temperatures) if

$$B \gtrsim B_0 \equiv \frac{100^2}{(2\pi)^2} \simeq 253. \quad (7)$$

For any choice of $\{n_r\}_{r=1..R}$, the canonical partition function will depend on how often solitons of exactly size n_r occur. We thus rewrite these configurations, now listing them using distinct integers n'_r with $n'_r > n'_{r+1}$ and the multiplicity $\#(n'_r)$ with which the value n_r had occurred:

$$\{n_r\}_{r=1..R} \longrightarrow \{(n'_r, \#(n'_r))\}_{r=1..R'}, \quad \sum_{r=1}^{R'} n'_r \#(n'_r) = N.$$

Note that replacing $\{n_r\}_{r=1..R}$ by $\{(n'_r, \#(n'_r))\}_{r=1..R'}$ is bijective, that is, to each set of n_r there is exactly one set of $(n'_r, \#(n'_r))$ (and vice versa); in the following we can thus always use the notation which is more convenient. The total canonical partition function is the sum

$$Z_{N, \text{total}}(\beta) \equiv \sum_{\substack{\{n_r\}_{r=1..R} \\ \sum_{r=1}^R n_r = N}} Z_{N, \{(n'_r, \#(n'_r))\}_{r=1..R'}}(\beta) \quad (8)$$

over the partition functions for fixed $\{n_r\}_{r=1..R}$

$$Z_{N, \{(n'_r, \#(n'_r))\}_{r=1..R'}}(\beta) = \prod_{r=1}^{R'} e^{-\#(n'_r)\beta E_0(n'_r)} Z_{n'_r, \#(n'_r), \text{kin}}(\beta), \quad (9)$$

² The many-particle ground state can be viewed as consisting of a relative wave-function given by a Hartree product state with N particles occupying the GPE-soliton mode $\propto \cosh[(x-x_0)/\sigma]^{-1}$ and a center-of-mass wave function for the variable x_0 (cf. [27, 50]). The one-body density matrix [48] then is $\propto \cosh[(x-x_0)/\sigma]^{-1} \cosh[(x'-x_0)/\sigma]^{-1}$ which vanishes in the limit $|x-x'| \rightarrow \infty$ even after integrating over x_0 . Thus, there is no off-diagonal long range order in our system.

where the kinetic part can be calculated using the recurrence relation [51] (which has been used to describe ideal Bose gases, e.g., in Refs. [52–54])

$$Z_{n_r, \#(n_r), \text{kin}}(\beta) = \frac{1}{\#(n_r)} \sum_{\ell=1}^{\#(n_r)} Z_{n_r, 1, \text{kin}}(\ell\beta) Z_{n_r, \#(n_r)-\ell, \text{kin}}(\beta), \quad (10)$$

with $Z_{n_r, 0, \text{kin}}(\beta) \equiv 1$ and the kinetic energy part of the single-soliton partition function is given by³

$$\begin{aligned} Z_{n_r, 1, \text{kin}}(\beta) &= \sum_{v=-\infty}^{\infty} \exp\left(-\beta \frac{E_{\text{gap}}}{n_r B N^2} v^2\right) \\ &\simeq \int_{-\infty}^{\infty} dv \exp\left(-\beta \frac{E_{\text{gap}}}{n_r B N^2} v^2\right) = \left(\frac{\pi n_r B N^2}{\beta E_{\text{gap}}}\right)^{\frac{1}{2}}. \end{aligned} \quad (11)$$

Rather than having to explicitly do sums over a large number (3) of configurations, for larger particle numbers it is preferable to calculate the partition function again via a recurrence relation, starting with $R = 1$ and $Z_{M, n_R, \#(n_R)}^{(R=1)}(\beta)$, $M = 1, 2, \dots, N$ given by Eq. (9). The step $R \rightarrow R+1$ then yields the case $n_{R+1} = n_R$ with

$$\begin{aligned} Z_{M+n_{R+1}, n_{R+1}, \#(n_{R+1})+1}^{(R+1)}(\beta) &= \frac{e^{-\beta E(n_{R+1})} Z_{n_{R+1}, \#(n_{R+1})+1, \text{kin}}(\beta)}{Z_{n_{R+1}, \#(n_{R+1}), \text{kin}}(\beta)} \\ &\times Z_{M, n_{R+1}, \#(n_{R+1})}^{(R)}(\beta) \end{aligned} \quad (12)$$

as well as

$$\begin{aligned} Z_{M+n_{R+1}, n_{R+1}, 1}^{(R+1)}(\beta) &= e^{-\beta E(n_{R+1})} Z_{n_{R+1}, 1, \text{kin}}(\beta) \\ &\times \sum_{n_R=n_{R+1}+1}^M \sum_{\#(n_R)=1}^{\lfloor M/n_R \rfloor} Z_{M, n_R, \#(n_R)}^{(R)}(\beta), \end{aligned} \quad (13)$$

where $\lfloor x \rfloor$ denotes the largest integer $\leq x$.

From the total canonical partition function (8) we obtain the specific heat (at fixed particle number N and system size L , which is proportional to the variance of the energy) as

$$\begin{aligned} C_{N,L}(T) &\equiv \frac{\partial}{\partial T} \langle E \rangle = -\frac{\partial}{\partial T} \frac{\partial}{\partial \beta} \ln[Z_{N, \text{total}}(\beta)] \\ &= \frac{1}{k_B T^2} \frac{\partial^2}{\partial \beta^2} \ln[Z_{N, \text{total}}(\beta)] = \frac{1}{k_B T^2} (\langle E^2 \rangle - \langle E \rangle^2); \end{aligned} \quad (14)$$

the number of atoms in the largest soliton is given by

$$\langle n_1 \rangle(T) = \frac{1}{Z_{N, \text{total}}(\beta)} \sum_{\substack{\{n_r\}, r=1..R \\ \sum_{r=1}^R n_r = N}} n_1 Z_{N, \{n_r, \#(n_r)\}}(\beta). \quad (15)$$

³ When approximating the sum $\sum_{v=-\infty}^{\infty} \exp(-xv^2)$ by the integral $\int_{-\infty}^{\infty} dv \exp(-xv^2)$, the error lies below 10^{-40} for $0 < x < 0.1$ [55]. When approaching the limit (4), $x \rightarrow 0$ and Eq. (11) thus becomes exact.

For analytic calculations Eq. (11) leads to

$$\begin{aligned} \frac{1}{[\#(n_r)]!} \left(\frac{\pi n_r B N^2}{\beta E_{\text{gap}}}\right)^{\frac{\#(n_r)}{2}} &\leq Z_{n_r, \#(n_r), \text{kin}}(\beta) \\ &\leq \frac{e^{\#(n_r)c_1}}{[\#(n_r)]!} \left(\frac{\pi n_r B N^2}{\beta E_{\text{gap}}}\right)^{\frac{\#(n_r)}{2}}, \quad c_1 \equiv \ln(2), \end{aligned} \quad (16)$$

the lower bound being (for temperatures large compared to the center-of-mass first excited state) the largest term involved in the sum (10); to obtain the upper bound we choose the value for c_1 such that all $2^{\#(n_r)-1} < e^{\#(n_r) \ln(2)}$ addends in the sum (10) (treated separately) are of the same order as the highest term.

In order to define a characteristic temperature (5), we now use the temperature below which finding a single soliton with N particles is more probable than finding N single particles. Both partition functions, evaluated at $T = T_0$, thus are the same,

$$Z_{N, 1, \text{kin}}(\beta_0) e^{-\beta_0 E(N)} = Z_{1, N, \text{kin}}(\beta_0), \quad \beta_0 \equiv \frac{1}{k_B T_0}. \quad (17)$$

While the left-hand side is known exactly [$Z_{N, 1, \text{kin}}(\beta)$ is given by Eq. (11)], the right-hand side of Eq. (17) lies between the bounds given by Eq. (16). Taking the N th root of Eq. (17) for each of these bounds leads [55], in the thermodynamic limit (4), to two characteristic, N -independent temperatures

$$T_1^{(\infty)} = \frac{2}{3} \frac{E_{\text{gap}}}{k_B} \frac{1}{W\left[\frac{8}{3} \pi B \exp(2)\right]}, \quad (18)$$

$$T_2^{(\infty)} = \frac{2}{3} \frac{E_{\text{gap}}}{k_B} \frac{1}{W\left[\frac{2}{3} \pi B \exp(2)\right]}, \quad (19)$$

where $W(x)$ is the Lambert W function which solves $W(x) \exp[W(x)] = x$ [55]. In the thermodynamic limit (4), the temperature for which it is equally probable to find N single particles and one bright soliton is lies in the range

$$0 < T_1^{(\infty)} \leq T_0^{(\infty)} \leq T_2^{(\infty)} < \infty$$

For numerical finite-size investigations we focus on particle numbers $N \approx 100$ relevant for generation of Schrödinger-cat states on timescales shorter than characteristic decoherence times [35]; $T_2^{(\infty)}$ turns out to be a characteristic temperature scale already for these particle numbers (see Fig. 1).

Figure 1 shows that the numerical data obtained via exact recurrence relations for the canonical partition function [Eqs. (9)–(13)]. at the transition many solitons are involved (Fig. 1 d). Near $T_2^{(\infty)}$, the numerical data is consistent with both the specific heat and the temperature-derivative of $\langle n_1 \rangle$ scaling $\propto N^2$ for $N \approx 100$.

To demonstrate that we indeed have a phase transition let us start by focusing on cases where we have $N - n$ particles in one soliton and n free particles; $n = O(N)$ and $N \gg 1$. Using Eq. (17) to express the partition function for n free particles corresponds to a system with fewer atoms (n) but the same g_{1D} thus rescaling E_{gap} and therefore also $T_{1,2}^{(\infty)}$ by a factor

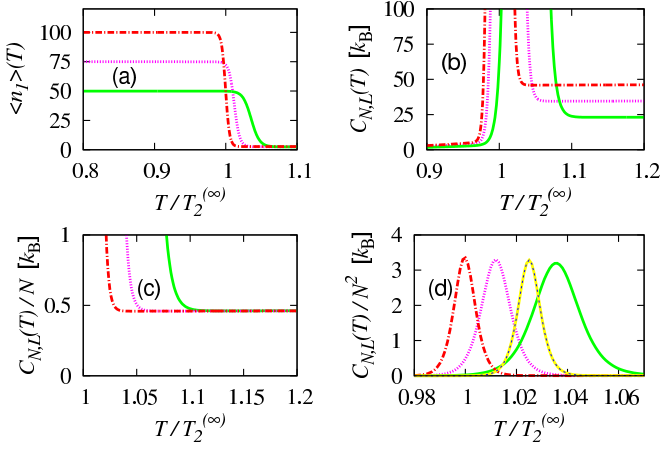


FIG. 1. (Color online) Finite size investigations of the soliton-non-soliton transition for $N = 50$ (green/gray solid line), $N = 100$ (red/black dash-dotted line) and $N = 75$ (magenta/gray dashed line) with $B = B_0$. (a) Size of the largest soliton (15) as a function of temperature. (b) For $N \approx 100$, the specific heat (14) as a function of temperature scales as $0.5k_B$ at low temperatures indicating one bright soliton. (c) At high temperatures, it scales as $\lesssim 0.5Nk_B$, demonstrating a free gas of N atoms. (d) The specific heat near the transition temperature scales as N^2k_B . Excluding all states with more than one soliton (yellow/light gray line, $N = 100$) clearly indicates the presence of several solitons near the transition temperature; the area of coexistence gets smaller for increasing N .

of $\frac{n^2}{N^2}$; the bounds in Eq. (16) now become for not too low temperatures

$$Z_{n,1,\text{kin}} \left(\frac{1}{k_B T_2^{(\infty)}} \right) \left(\frac{T}{T_2^{(\infty)} \frac{n^2}{N^2}} \right)^{\frac{n}{2}} \exp \left(\frac{(n+1)E_{\text{gap}}}{3k_B T_2^{(\infty)}} \right) \leq Z$$

$$\leq Z_{n,1,\text{kin}} \left(\frac{1}{k_B T_1^{(\infty)} \frac{n^2}{N^2}} \right) \left(\frac{T}{T_1^{(\infty)} \frac{n^2}{N^2}} \right)^{\frac{n}{2}} \exp \left(\frac{(n+1)E_{\text{gap}}}{3k_B T_1^{(\infty)}} \right), \quad (20)$$

with $Z = Z_{1,n,\text{kin}}(\beta)$ and $T_2^{(\infty)} > T_1^{(\infty)}$. Multiplying this equation with $\exp[-\beta E_0(N-n)]$ to obtain the full partition function with $N-n$ particles in one soliton and n free particles and dividing by $\exp[-\beta E_0(N)]$ yields that for $n \approx N$ the n -dependence (and in particular the question if they grow or shrink) is dominated by the $(T/T_{1,2}^{(\infty)})^{n/2}$ -terms. Including factors of the order of (3) to include the contribution of all other configurations with $N-n$ particles in one soliton (or directly including terms with more than one small soliton) does not change the convergence behavior. Summing over $n \approx N$ such that the sum includes a finite fraction of N , say, all $n \geq 0.99N$, we thus have

$$0 < \lim_{N \rightarrow \infty} \frac{\langle n_1 \rangle}{N} \leq 1, \quad T < 0.99^2 T_1^{(\infty)}. \quad (21)$$

Extending the above reasoning based on Eq. (20) to high temperatures ($T > T_2^{(\infty)}$) shows that in the sum (15):

$$\lim_{N \rightarrow \infty} \frac{\langle n_1 \rangle}{N} = 0, \quad T > T_2^{(\infty)}. \quad (22)$$

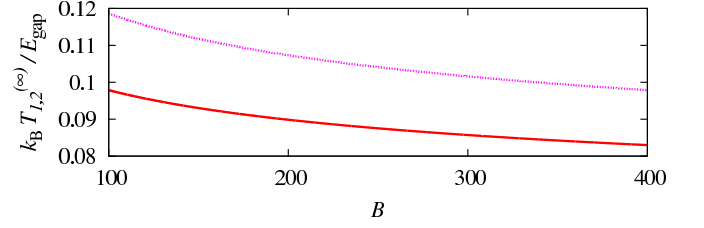


FIG. 2. (Color online) Characteristic temperatures for the soliton-non-soliton transition in the thermodynamic limit (4) as a function of B [Eq. (6) which depends on the ratio of the system size and the size of a two-particle soliton.]. Upper, magenta/gray dotted curve: above this temperature, the relative number of atoms in the largest soliton vanishes [Eq. (22)]. For temperatures below the red/black solid curve, a macroscopically occupied bright soliton exists [Eq. (21)]. The transition region is small compared to the difference of the two curves (cf. Fig. 1).

Thus, using the canonical ensemble [49] we have shown the existence of a phase transition in the thermodynamic limit (4) [cf. Fig. 2].

The N -dependence of the specific heat shows that both in the high-temperature phase [Fig. 1 (b),(c)] and in the low-temperature phase [Fig. 1 (b)] predictions of the canonical and the microcanonical ensemble [49] agree [49]. As the mean energy is a monotonously increasing function of temperature [Eq. (14)] and as furthermore, the choice of the thermodynamic limit (4) leads to a mean energy $\propto N$ and an N -independent temperature scale, the $\propto N^2$ behavior displayed by the specific heat in Fig. 1 (d) can only occur in a small ($\propto 1/N$) temperature range in which both ensembles no longer are equivalent.

To conclude, we find the existence of a finite-temperature many-particle phase transition in a one-dimensional quantum many-particle model, the homogeneous Lieb-Liniger gas with attractive interactions [Eqs. (21) and (22); Fig. 2]. The low temperature phase consists of a macroscopic number of atoms being one large quantum matter-wave bright soliton with delocalized center-of-mass wave function (which does not display long-range order thus not violating the Mermin-Wagner theorem [13, 14]; the Landau criterion [56] which argues against the co-existence of two distinct phases is also not violated); the high temperature phase is a free gas. As a harmonic trap would facilitate soliton formation [58], we conjecture that the existence of a finite-temperature phase transition remains true for weak harmonic traps. In experiments, even the *integrable* Lieb-Liniger gas can thermalize as the wave guides are *quasi*-one-dimensional (cf. [11, 12]).

Via exact canonical recurrence relations we also numerically investigate the experimentally relevant case of some 100 atoms (cf. [5, 35, 36]) with the (experimentally realizable [44]) box potential. The spike-like specific heat provides further insight: the specific heat ($\propto N^2$) is the derivative (14) of an energy scaling not faster than $\propto N$ (4). At low temperatures all atoms form one soliton; the size of the soliton thus is an ideal experimental signature (cf. [1–10]).

I thank T. P. Billam, Y. Castin, S. A. Gardiner, D. I. H. Holdaway, N. Proukakis and T. P. Wiles for discussions and the UK EPSRC for funding (Grant No. EP/L010844/1 and EP/G056781/1). The data presented in this paper will be available online [59].

Note added: Recently, a related work appeared [60].

* christoph.weiss@durham.ac.uk

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